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Predictive sysytem of a chemical joint: Surface Energy calculation

One of the main issues in adhesive technology is the appropriate choice of the joint suitable for the material of interest that must provide the best holding of the system.

The aim of this work is the ab initio estimate of the Adhesion compatibility

The study of the surface energy of a material can be a good parameter.

From an experimental point view techniques based on the determination of the contact angle and friction are presented.

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Surface energy and surface tension: a quick overview view

In the all-day language surface energy and tension are often confused and not used in the correct way.

The first one refers to solids while the second one to liquids.

Let's start from thermodynamic: all the systems tends to their minimum energy.

In our particular case the system is composed by molecules (of the substrate and the tape for example) and the energy is determined by intermolecular interaction.

Considering an isolated solid, surface energy is defined as the energy related to the disruption of intermolucar bonds when the surface itself is created, since the molecules on top of the material lose some of them.

In other terms it can be seen as the excess energy of the surface with respect to the bulk of the material.

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If we consider an isolated liquid, for example a droplet in vacuum, for the same energetic reason it will tend to minimize its ratio surface/bulk and this is realized smoothing its shape: that's why the droplet's form.

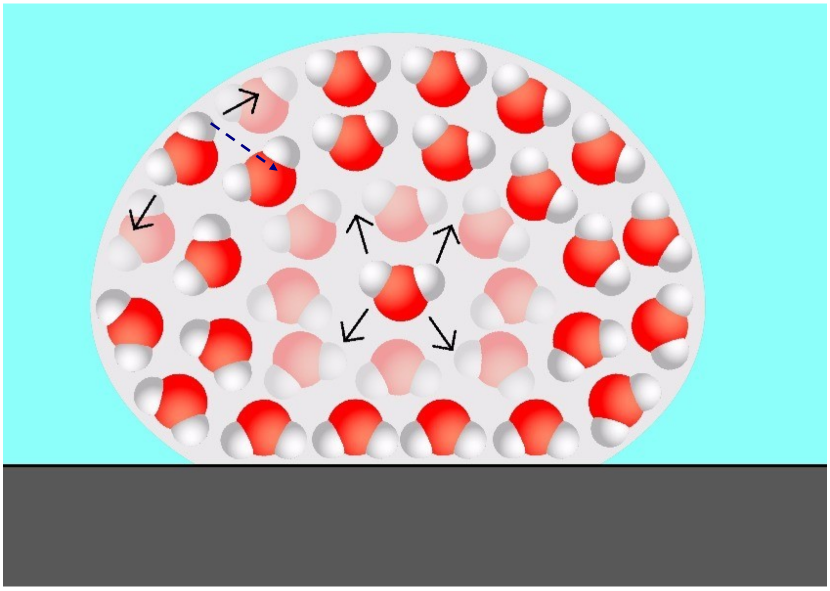

Figure 1: Molecules in the bulk interact with their neighbours in all directions while the surface ones' experience a net attraction to the intern that give rise to the surface tension

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Wetting phenomena: Interfacial energy

Now let's complicate our system of study and bring the solid and the liquid in contact and consider the simplest example of a water droplet on a solid.

We must always remind the tendency of all system to their energy minimum.

Let's call E_{l-l} and E_{s-l} the intermolecular bond energy between two liquid molecules and between a liquid and a solid molecules respectively.

What happens reminding that a liquid alone would form a sphere?

We have to distinguish some cases.

If $E_{l-l} > E_{s-l}$ (we are considering the absolute value since interaction energy has always negative sign) liquid molecules tends to maximize the number of l-l interactions with respect to s-l bonds and so they will form sherical droplets on top of the surace.

What is commonly said is that the surface is hydrophobic.

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Experimental technique: Contact angle

In the case of $E_{l-l} < E_{s-l}$ instead liquid molecules will tend to maximize the number of s-l interactions and the liquid will wet the surface.

What is commonly said is that the surface is hydrophilic.

For a general liquid the degree of wetting is relative to the solid substrate.

The degree of wetting depends on the difference between E_{l-l} and E_{s-l} and can be parametrized with a measure of contact angle.

This quantity is defined as the angle between the liquid surface's tangent and the substrate.

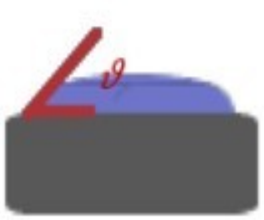

Figure 2: Contact angle ϑ

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Experimental technique: Contact angle

It is well known that contact angle measurments give a rapid and inexpensive idea of the ratio E_{l-l} / E_{s-l} since the greater is the angle the higher will be the degree of "hydrophobicity".

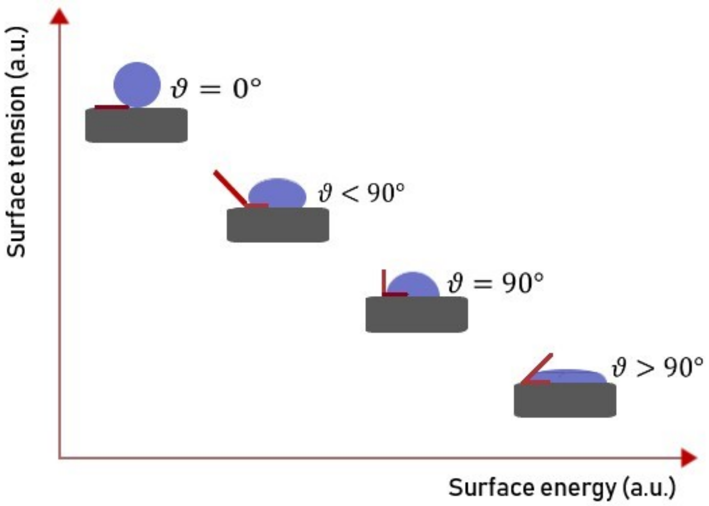

Figure 3: General rule of thumb to estimate the wetting capability

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Experimental technique: Roll-Off angle

This method is clearly not enough precise to predict the adaptability of a tape with a substrate.

It would be possible to exploit available tables with values of surface energy and tension but for real-life studies does not faces pure and cleaned surfaces but instead dirty and/or treated ones, That's why a rapid, economic and well reproducible method is needed.

While the measure of the contact is about a static condition of the system we can think of perform a dynamical one: the roll-off angle.

It is defined as the smallest angle needed to put in motion the droplet on the substrate of interest.

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Experimental technique: Roll-Off angle

Actually the geometry of the system allows to define two variables: the back-contact angle and front-contact angle that together provide the measure of the droplet's hysteresis.

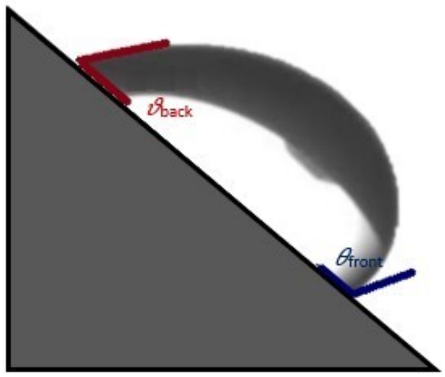

Figure 4: Droplet's hysteresis

Actually the geometry of the system allows to define two variables: the back-contact angle and front-contact angle that together provide the measure of the droplet's hysteresis.
The deformation is due to the effect of both cohesive forces of the liquid and adhesive forces that tend to prevent the rolling opposing the gravity.

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Experimental techinque: Friction measure

To increase the number of parameters under control it is useful to evaluate the static and dynamic friction coefficients.

The first one is directly determined, with simple physics' calculation by the roll-off angle configuration.

The second quantity, instead, is a more tricky one and needs a dynamic measure to write the law of motion of the droplet from which the dynamic friction coefficient can be evaluated.

This is done using a tracking-image software.

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Surface adaptability study: mechanical tests

Now there are two ways to go on with the study.

First of all let's image to fix the liquid and to perform the measurments described before. We end up with a set of parameter related to the surface energy of the substrate on study.

Let's add the tape, perform mechanical stress test (like for example the peel test) and collect the results.

A lot of variables comes into play and the duty of the sperimenatalist is to keep fixed the highest number of them in order to get meaningful results.

Performing these tests for many tapes we can construct an inside database of "surface energy vs response to tape x".

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Surface adaptability study: surface energy

The second line of reasoning would respond to the following question: “Is it possible to measure the surface tension of an adhesive so that it could be compared to the surface energy of a target substrate?”.

Let’s remind that adhesion depends on the kind and on the intensity of the interaction between molecules of the tape and of the surface.

Besides different tapes can exhibit pretty wide different viscoelastic behaviour that can affect their capability of bonding to different surface geometry.

Collecting enough data of the previously explained measurments with different liquid would make possible to test if there is or not a ready-to-use rule for adaptability.

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Conclusions

As a rule of thumb we can say that in the presence of an high surface energy (HSE) a wider range of adhesive will be performant with respect to a low surface energy (LSE).

It must be said that in this report a lot of parameters that influence the adhesion like roughness, pre-tretreatment, dirty and so on have not been taken into account with precise attention.

Anyway the method proposed circumvent their characterization stacking their influence in some easy-to-measure parameters which furthermore provide a way to detect a problem in an unexpected result (for example if all the processing parameters of two substrate made of the same material are proven to be the same but the contact angle is different it is probable that some kind of contaminant is present).

As said before further improvement will depend on the capability to realize a scale of surface tension for the adhesive materials.

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